DRAFT

Application of the Loci-based CFD code Chem at MSFC: Preliminary Results

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Outline

1. *Objectives*
2. *What is the Loci-Chem CFD code?*
3. *Application to Bifurcating Duct problem*
4. *Application to Single Element Injector*
5. *Application to PSU RBCC rig*
6. *90 degree Elbow Benchmark problem*
7. *Future Work*

Objectives

1. Determine what class(es) of simulations the Loci-Chem code can handle at this point (Loci-Chem is still a Beta release)
2. Perform a quick survey, not a rigorous validation study
3. Concentrate on determining the qualitative accuracy, performance and robustness of the Chem code

What is the Loci-Chem CFD Code?

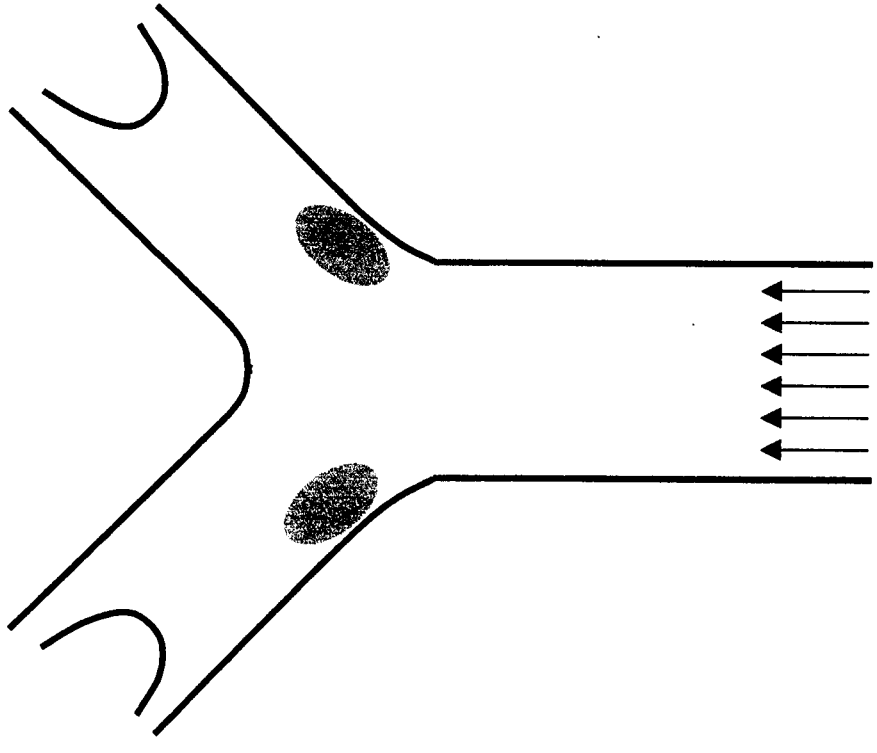
Developed by Ed Luke and P. Cinnella at Mississippi State University, since 1998.

- Density-based, finite volume, generalized unstructured grid, Navier-Stokes solver
- The original intent of the algorithm is to provide high performance finite rate chemistry computations
- The algorithm was implemented using the Loci framework, which allows implementation issues such as parallel processing to be handled transparently to the coding of the CFD algorithm
- The Loci-framework allows reduced-labor multi-disciplinary applications, for example, CFD plus solid-phase finite element analysis

Comparison of Chem and FDNS on Bifurcating Duct

Bifurcating Duct

- Flow splits from single duct to two ducts
- Flow restrictions exists at the exit of the smaller ducts
- Separated regions occur on the outboard side of the flow split



Motivation to use Chem

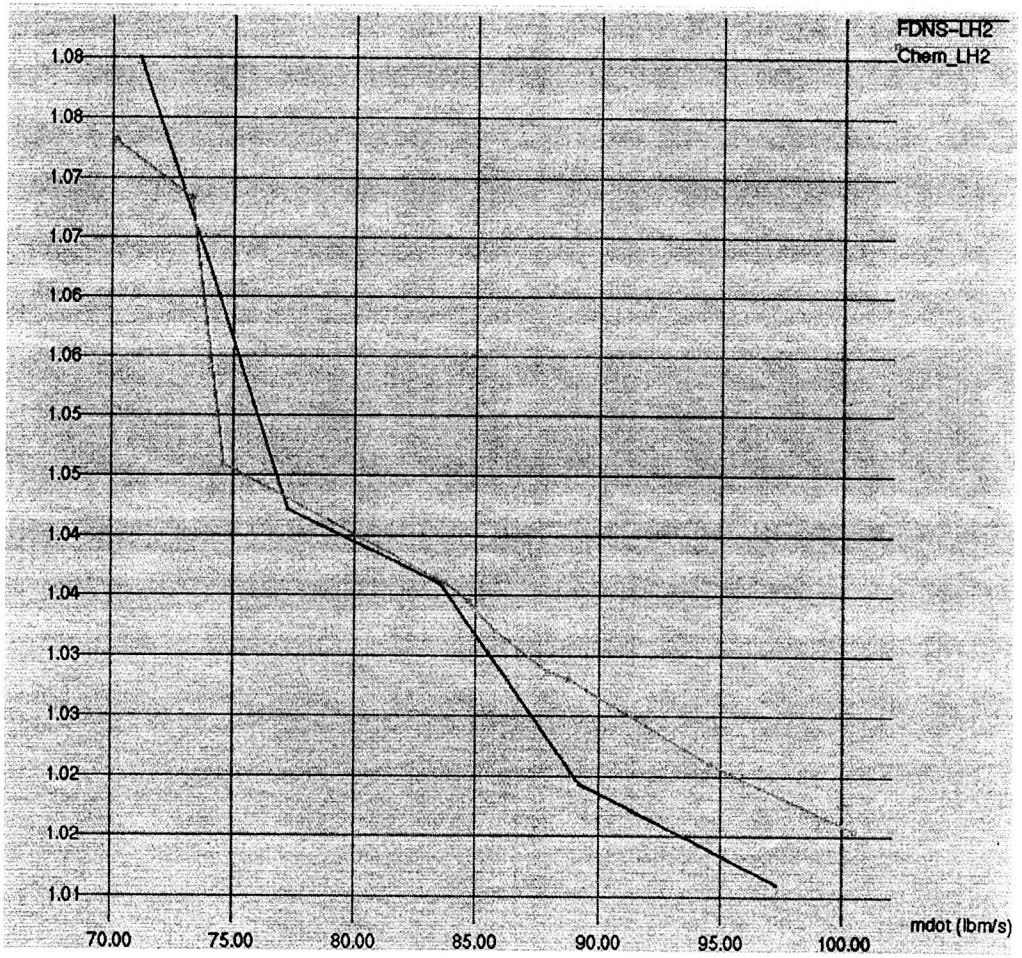
- Structured grid became very large
- FDNS approaching scalability limit
- ***Are Chem predictions consistent with FDNS predictions?***

Predicted Blockage from Chem and FDNS

Bifurcating Duct, Structured grid

- X-axis: mass flow rate through duct
- Y-Axis is blockage, >1 means separation is present
- Red Line is FDNS results
- Green line is Chem results
- Results compare favorably

- Grid is not appropriate for Chem turbulence model
- Pressure losses do NOT agree, will address later



Performance of Chem and FDNS on Bifurcating Duct

Chem

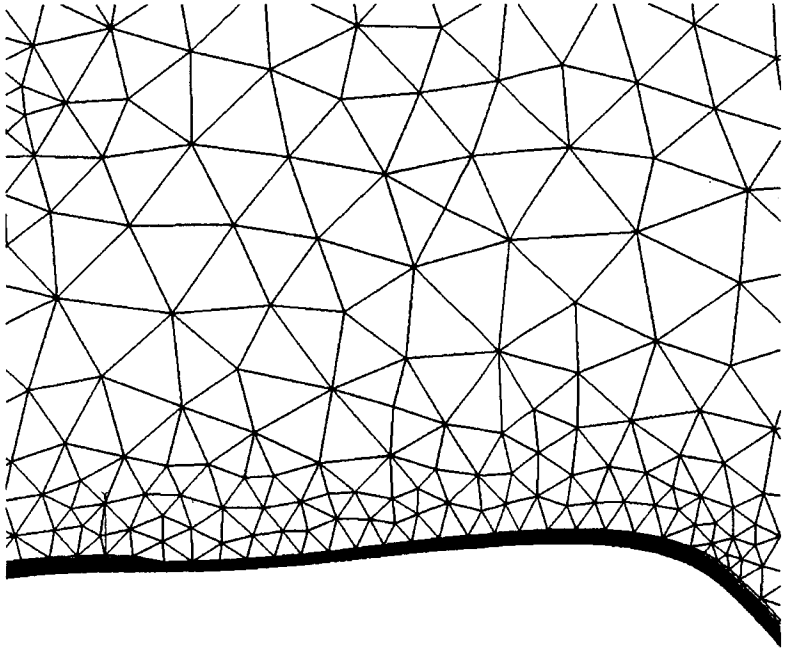
- 0.541M grid points
- 6 hours wall clock using 17 CPUS
- 4.25 CPU days total effort
- Max possible CPUs for quality result=unknown. MSFC has used up to 52 CPUs on a single task. Difficult to find more than 52 CPUs due to heavy use of MSFC PC Cluster.

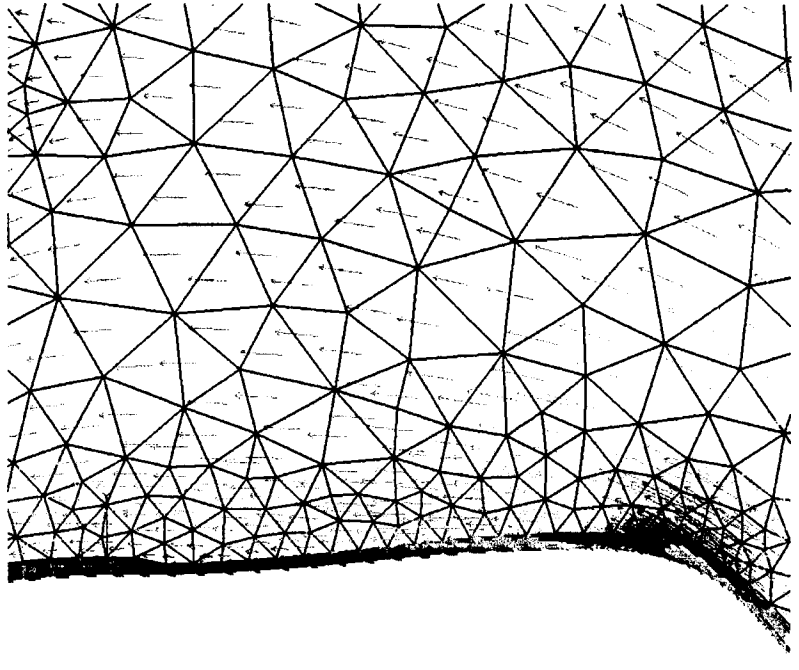
FDNS

- 0.541M grid points
- 3 days wall clock using 4 CPUs
- 12 CPU days total effort
- Max possible CPUs for quality result=4, due to grid constraints.

Performance of Chem with Hybrid grids on Bifurcating Duct

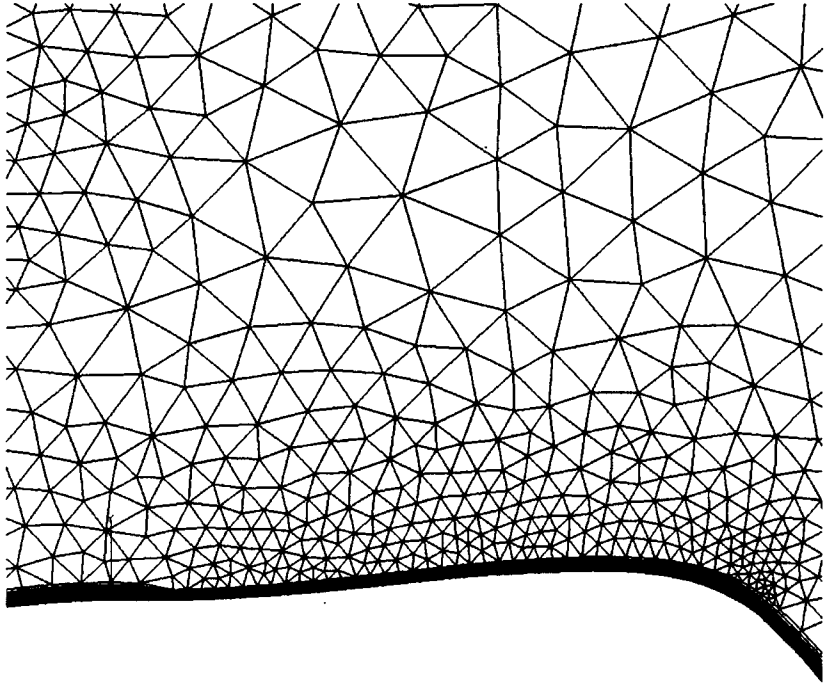
Convergence and mass conservation were similar to the structured grid, however, the large separated region disappeared

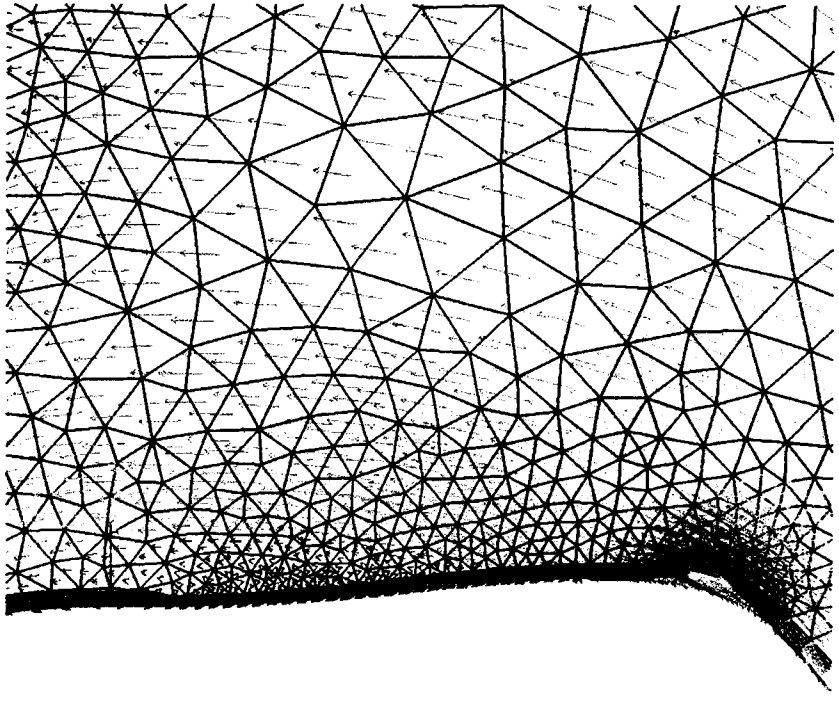




Performance of Chem with Hybrid Grids on Bifurcating Duct

The large separated region appeared after refining the unstructured grid in the transition from structured to unstructured



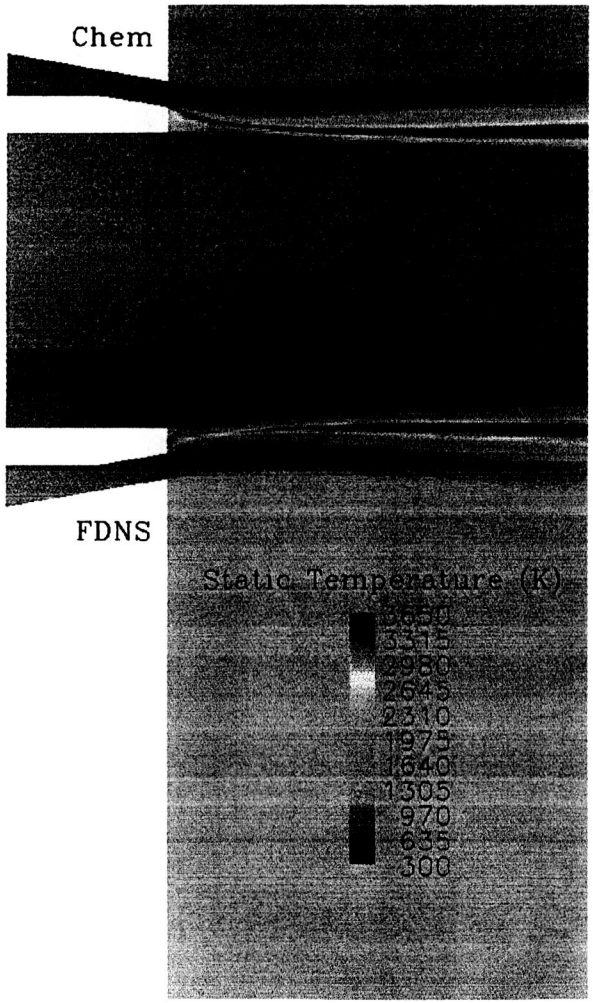


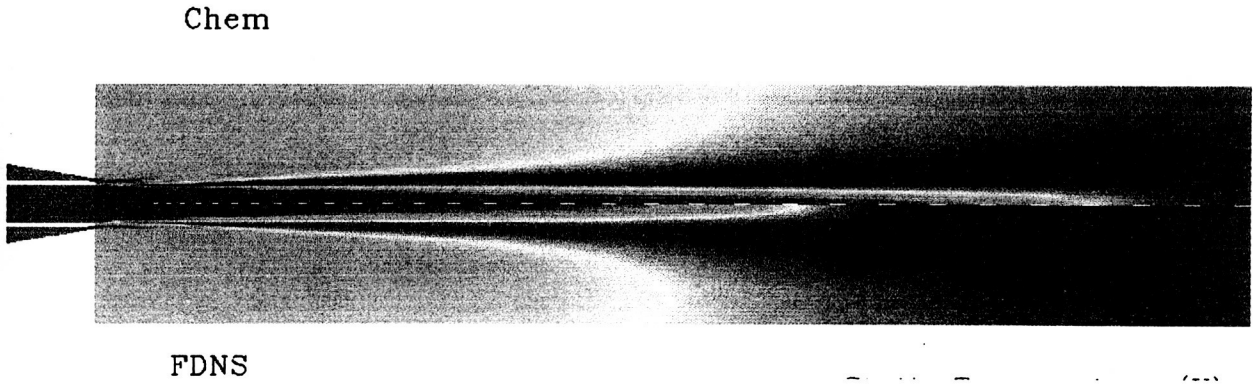
Predictions of Chem and FDNS on Single Element Injector

Case 26 from SCIT Task optimization suite

- Gaseous Oxygen/Gaseous Hydrogen
- Axisymmetric geometry
- O/F=4.0
- Pc=750 psia?

Predictions of Chem and FDNS on Single Element Injector

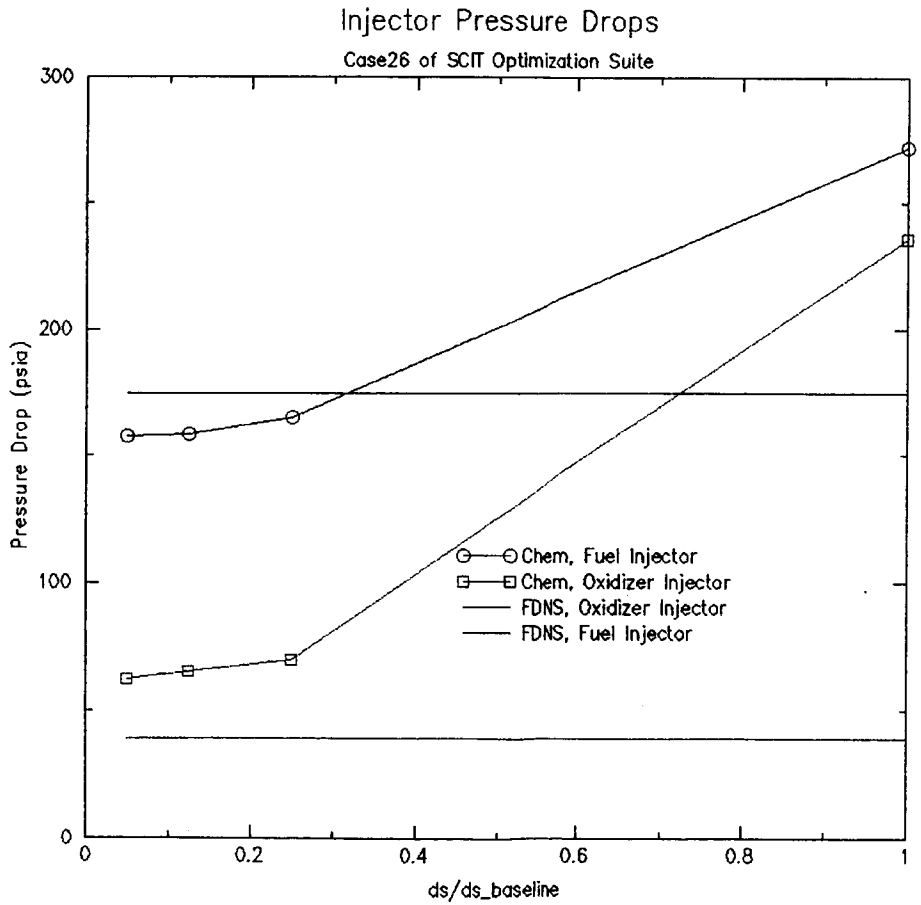




Comparison of Temperature Fields

- Combustion length is different
- Codes differ in turbulence models, thermodynamic property models, and reaction kinetics, each difference can be evaluated in turn

Predictions of Chem and FDNS on Single Element Injector- Injector Pressure Drops



Comparison of injector pressure drops

- Grid-independent pressure drops from Chem
- FDNS pressure drops are probably near grid-independent
- Reasonable first comparison, more work required

Performance of Chem and FDNS on Single Element Injector

Chem

- 74,810 grid points
- 7 hours wall clock using 22 CPUS
- 6.5 CPU days total effort
- Max possible CPUs for quality result=?. MSFC has used up to 52 CPUs on a single task. MSU-ERC has used up to 128 CPUS on a single task.

FDNS

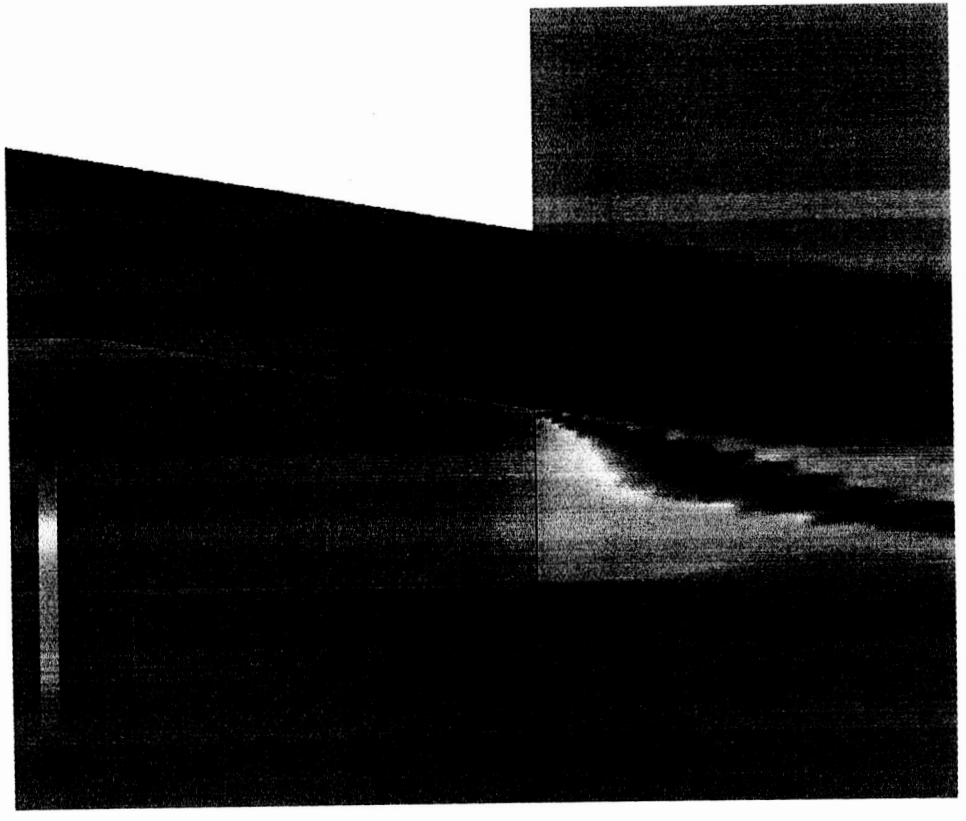
- 34830 grid points
- 5 days wall clock using 1 CPUs
- 5 CPU days total effort
- Max possible CPUs for quality result=1, due to grid constraints.

Performance of Chem and FDNS on Single Element Injector- Conjugate Heat Transfer

Conjugate Heat Transfer

- Solid-phase control volume approach
- Dynamic link library contained the new application, only a few lines of code in the main application required changing
- User Creates grid and input file, adds an option to code invocation
- Parallel operation is automatic through Loci framework

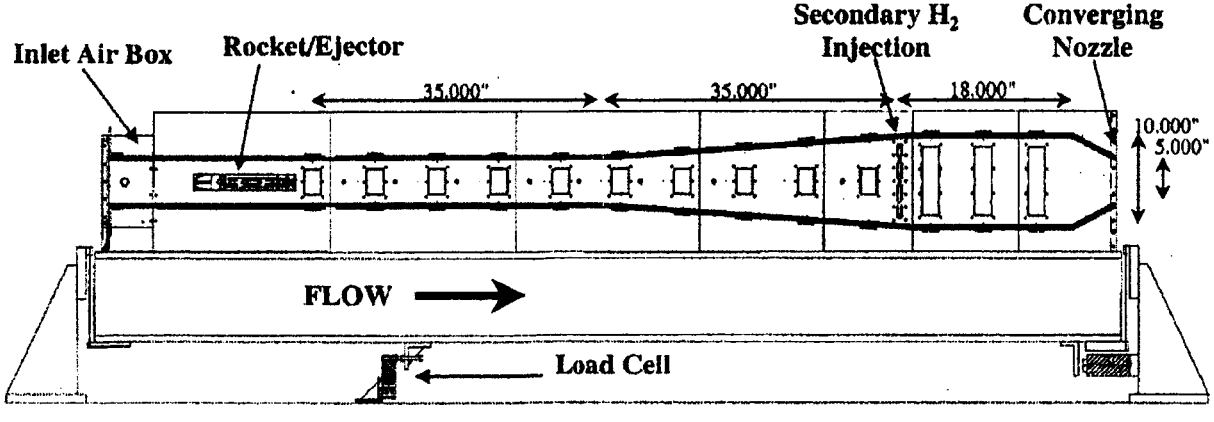
Static Temperature in K for both solid and gas phases



Application to PSU RBCC rig

DC, SR500, Case 3

- Direct connect air-flow configuration
- 500 psia single rocket (GH2/GO2)
- Ram Fuel (GH2) Injection Activated
- Model using 2 symmetry planes



Case 3 Operating Conditions

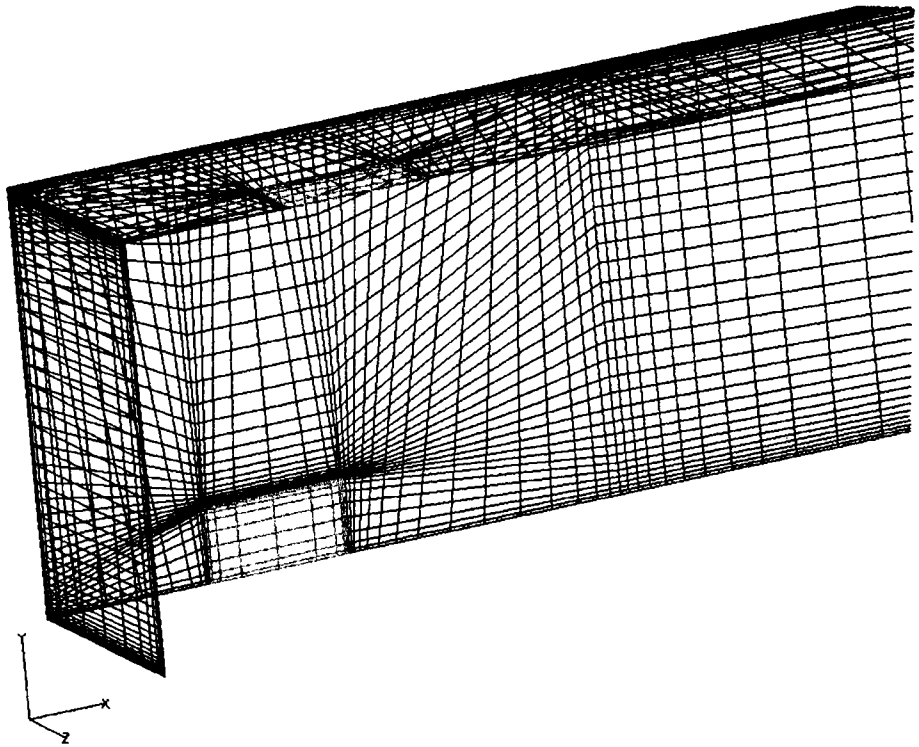
Rocket	
O/F	8.0
Pc (psia)	500
Mass Flow Rate (lbm/s)	0.684
Duct	
Mass Flow Rate of air (lbm/s)	1.575
Mass Flow Rate GH2 (lbm/s)	0.046
O/F	8.0

Application to PSU RBCC rig

Existing Grid Details

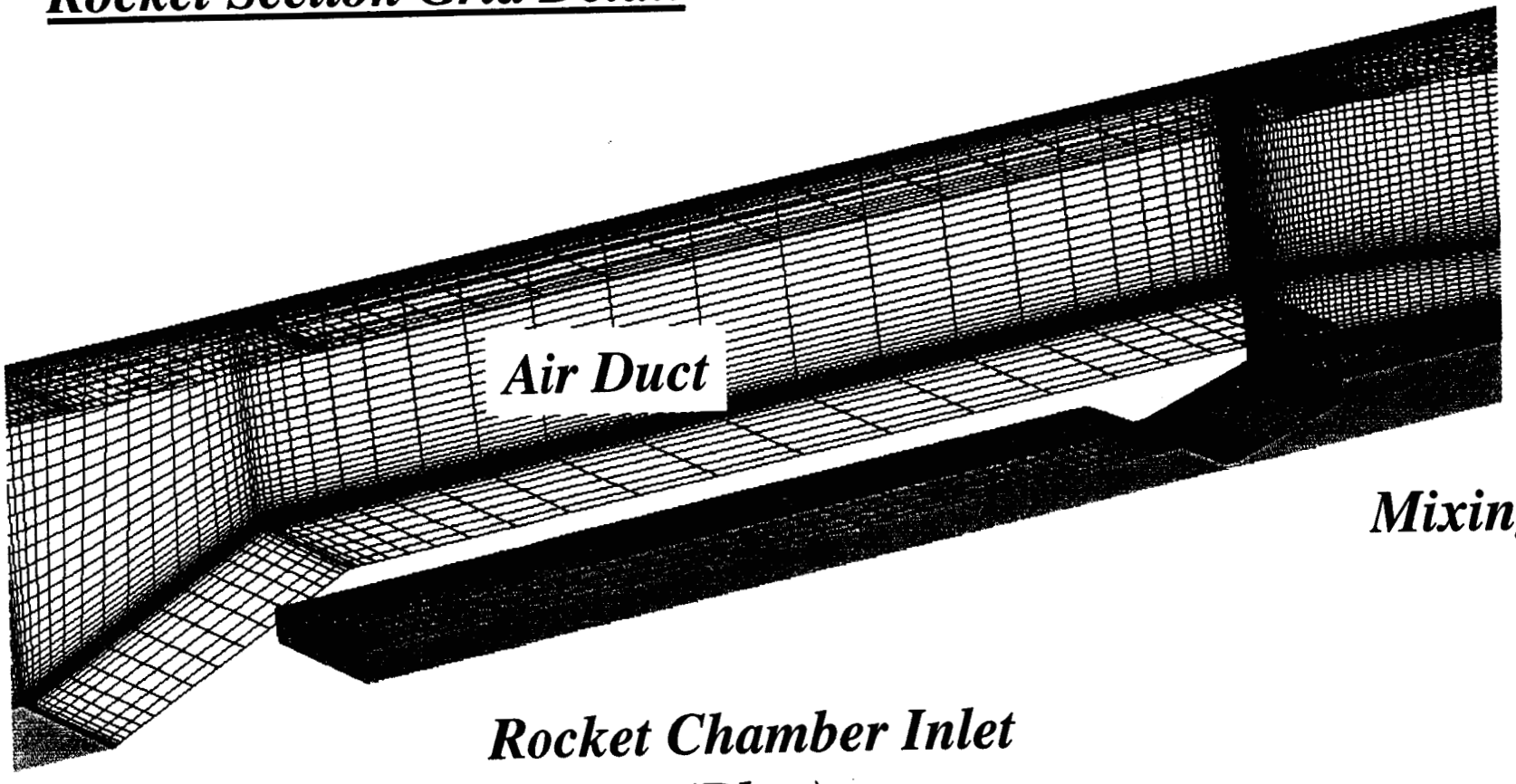
- *3 Structured grid sections (0.6M pts)*
  - *(131x45x15) - Air Duct (14%)*
  - *(413x85x15) – Mixing Duct(80%)*
  - *(131x21x15) – Rocket(6%)*

Direct-Connect Inlets (Green)



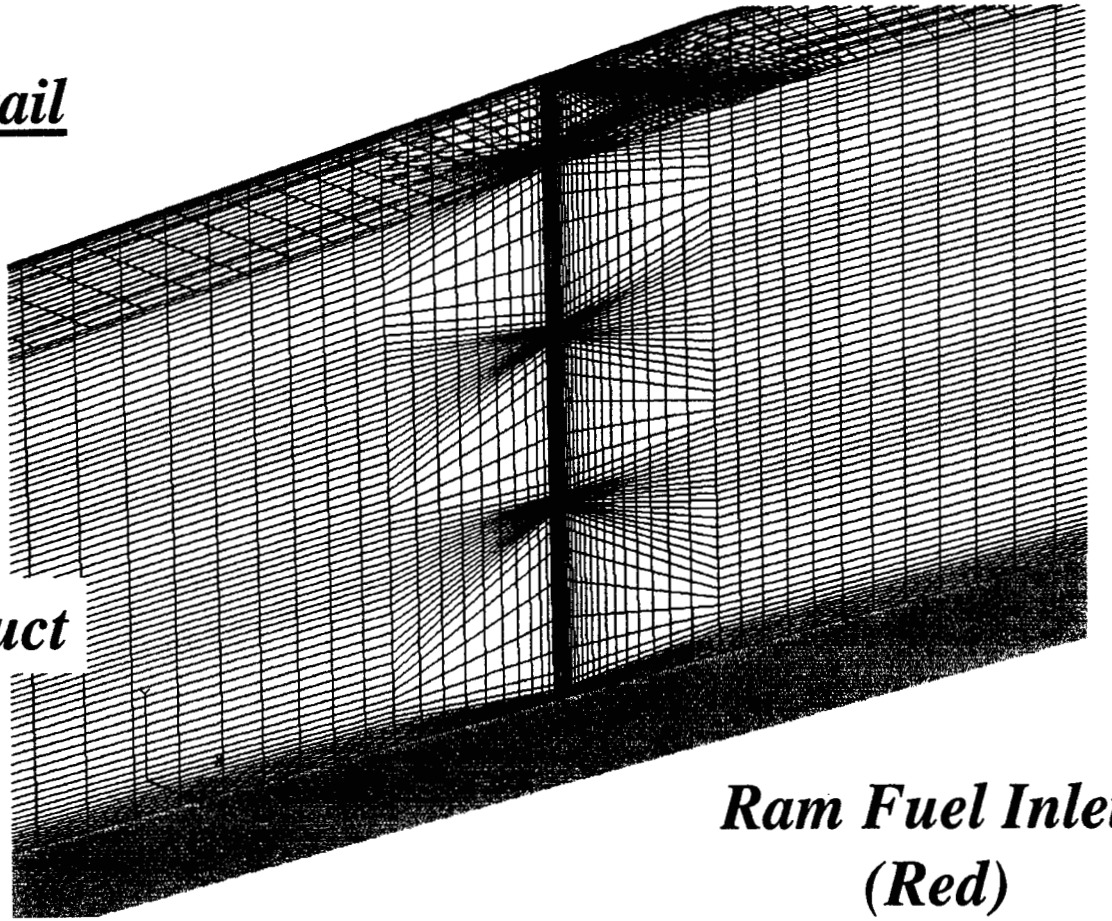
Application to PSU RBCC rig

Rocket Section Grid Detail



Application to PSU RBCC rig

Ram Section Grid Detail



Mixing Duct

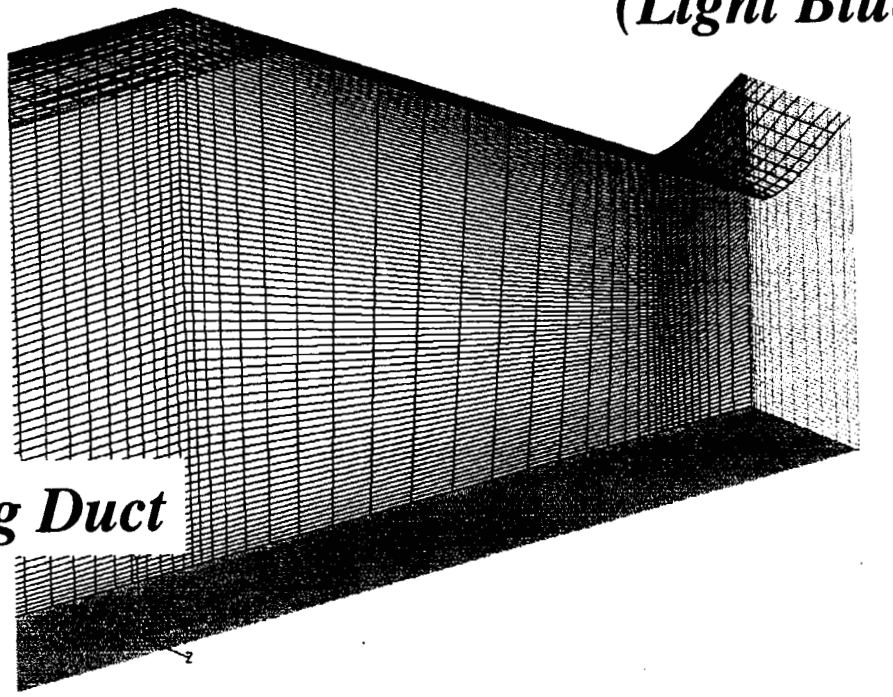
Ram Fuel Inlets (Red)

Application to PSU RBCC rig

Outlet Section Grid Detail

- *Ambient conditions with characteristic BC*
- *Throat is not choked*
- *Previous experience has shown need to model outlet ambient region*

Outlet BC Surface (Light Blue)



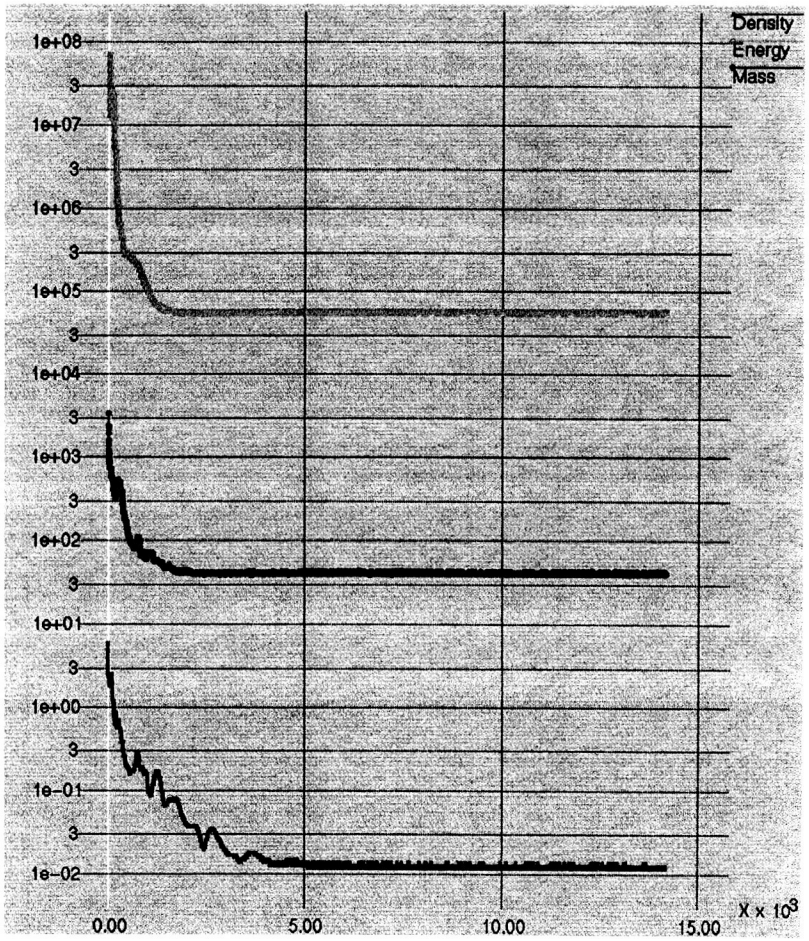
Mixing Duct

Application to PSU RBCC rig

Simulation Details

- *Used 32 CPUs (mix of 600 and 933 MHz PIIIs)*
- *Started with ICs of quiescent air using frozen chemistry*
- *Ran 14,000 iterations in 9 days*
- *Achieved from 2 to 3 orders of magnitude reduction in residual*
- *Computational domain mass conservation within 0.015%*

Residuals

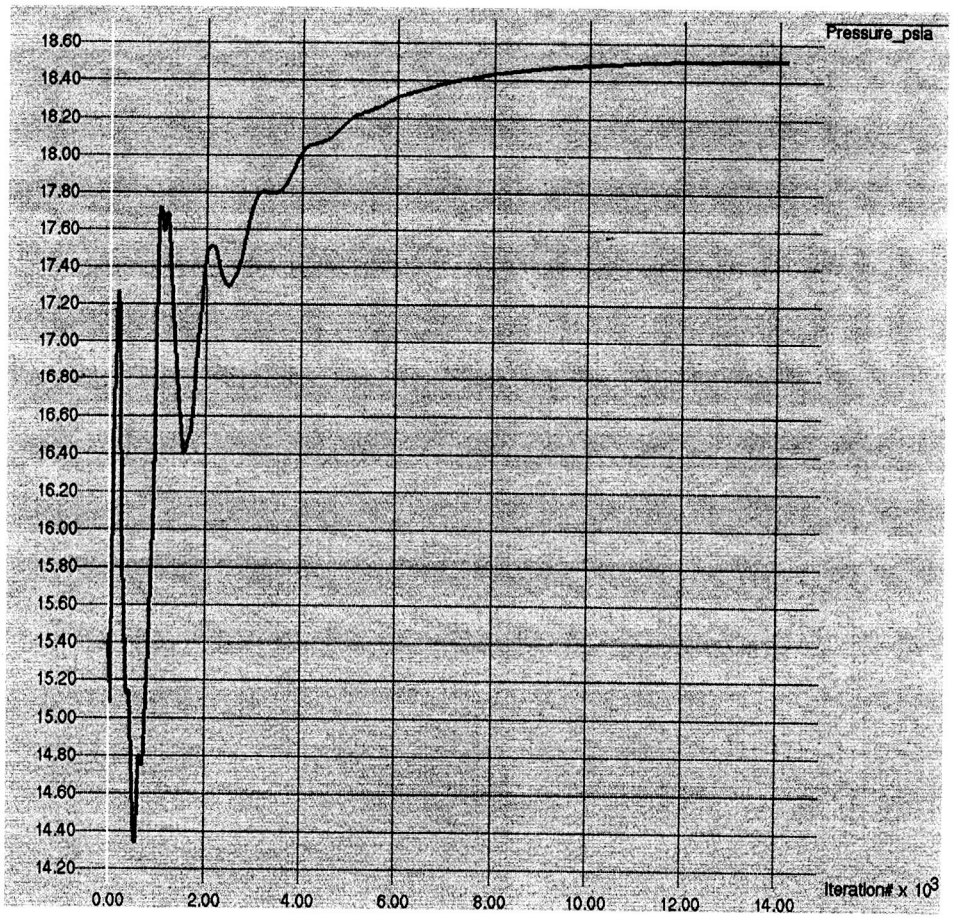


Application to PSU RBCC rig

Pressure vs. Iteration number

Simulation Details

- ***Pressure in head end of Air Duct was slow to converge***
- ***It finally converged, but the time required seems to great***
- ***It may be that the timestep setting was too conservative***
- ***The Timestep was set to 1e-5 seconds, the value that allowed the simulation to develop from quiescent conditions***

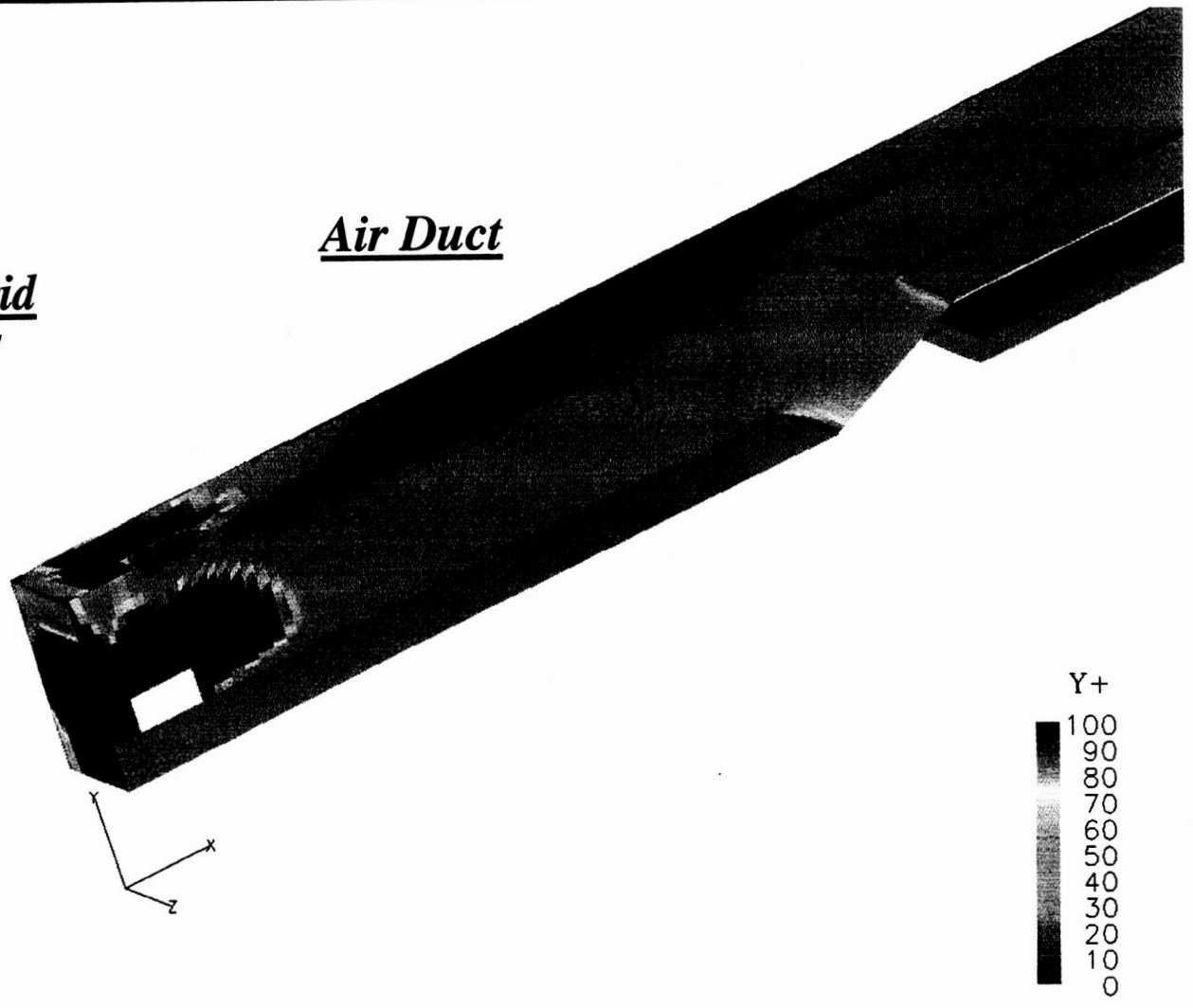


Application to PSU RBCC rig- Y+ values

Y+ values for existing grid

- *Values over 100 are red*
- *Only small regions are acceptable*

Air Duct

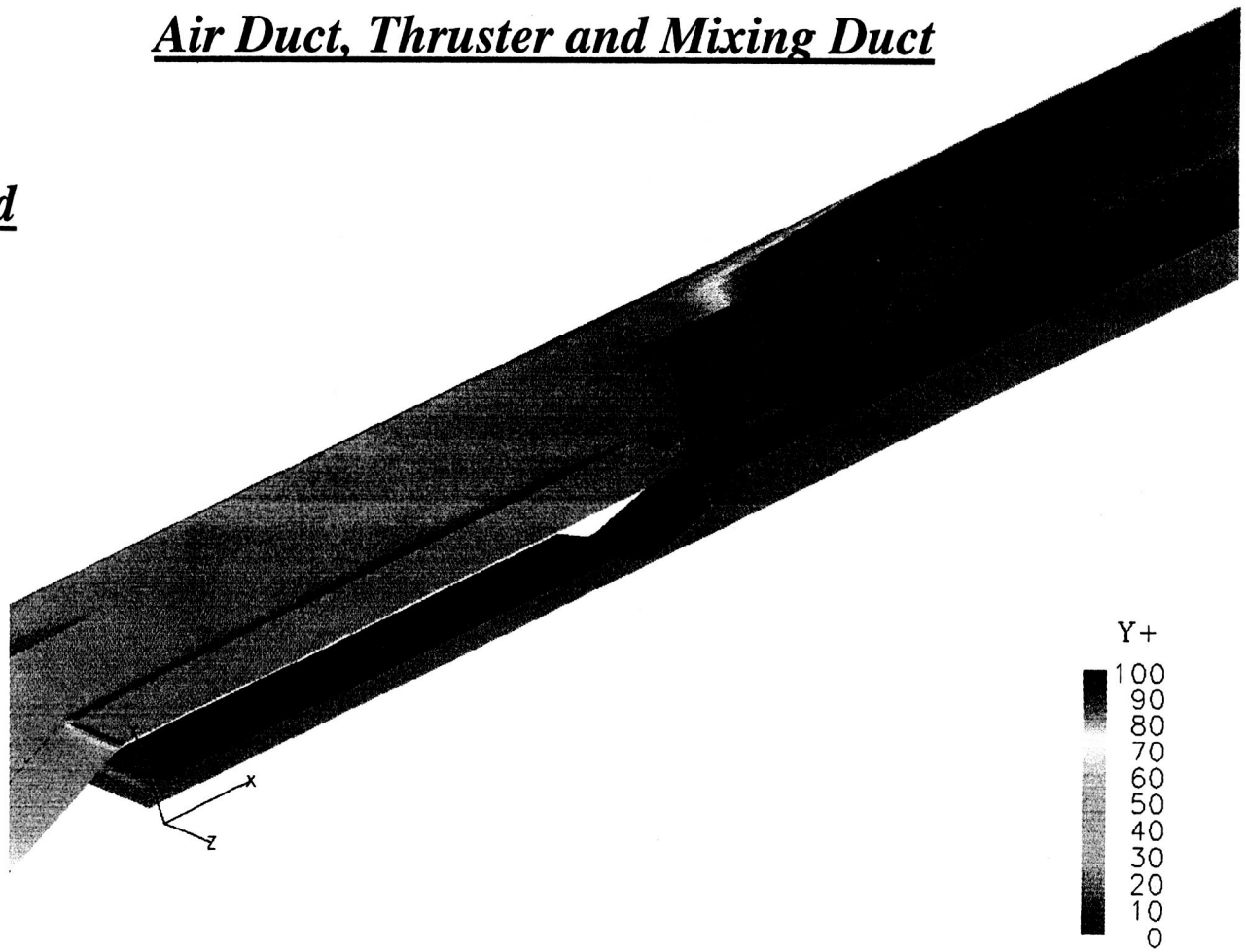


Application to PSU RBCC rig- Y+ values

Air Duct, Thruster and Mixing Duct

Y+ values for existing grid

- ***Values over 100 are red***
- ***Only small regions are acceptable***
- ***The rocket top surface appears to be acceptable***

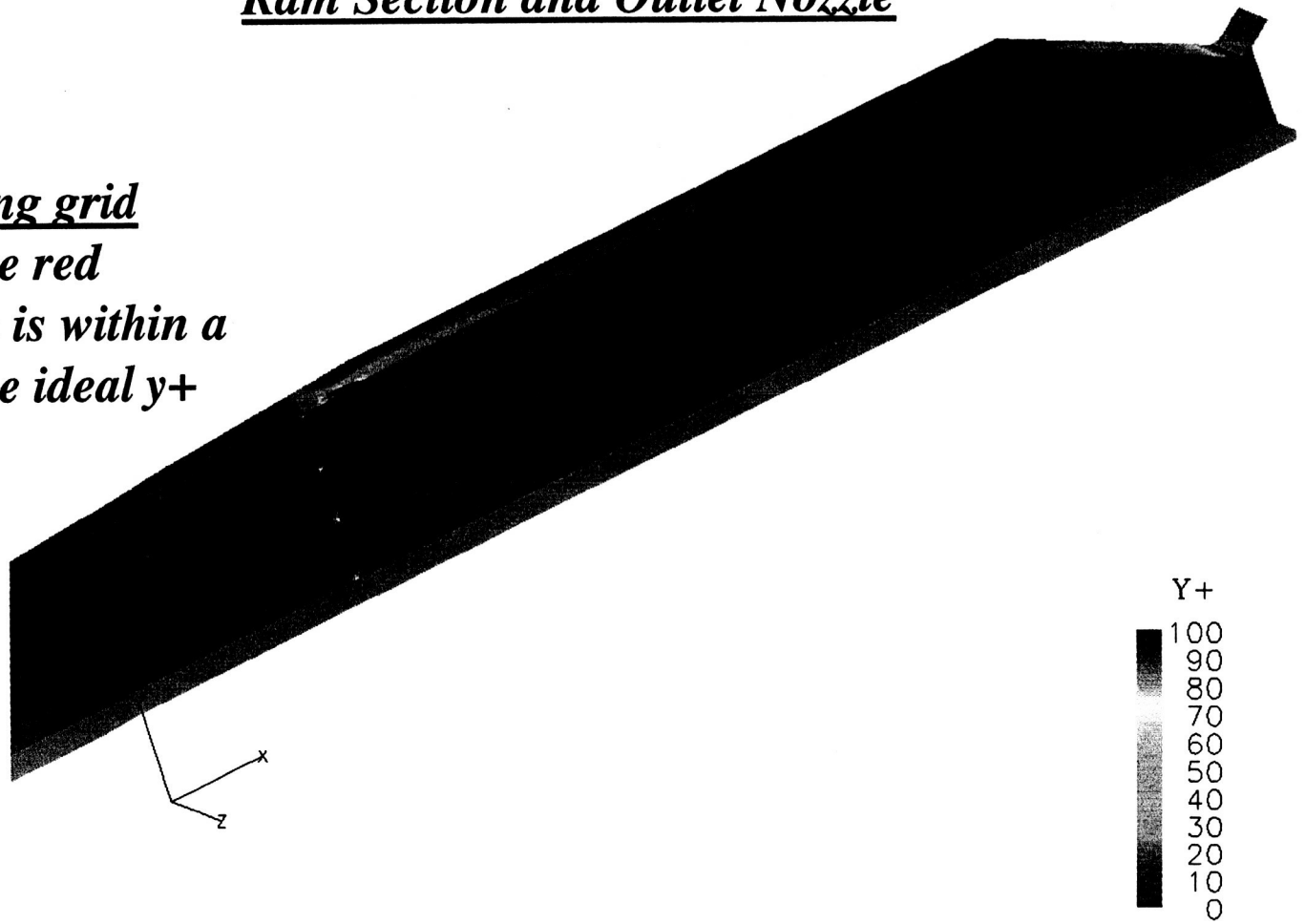


Application to PSU RBCC rig- Y+ values

Ram Section and Outlet Nozzle

Y+ values for existing grid

- *Values over 100 are red*
- *Most of this region is within a factor of 20 from the ideal y+ values*

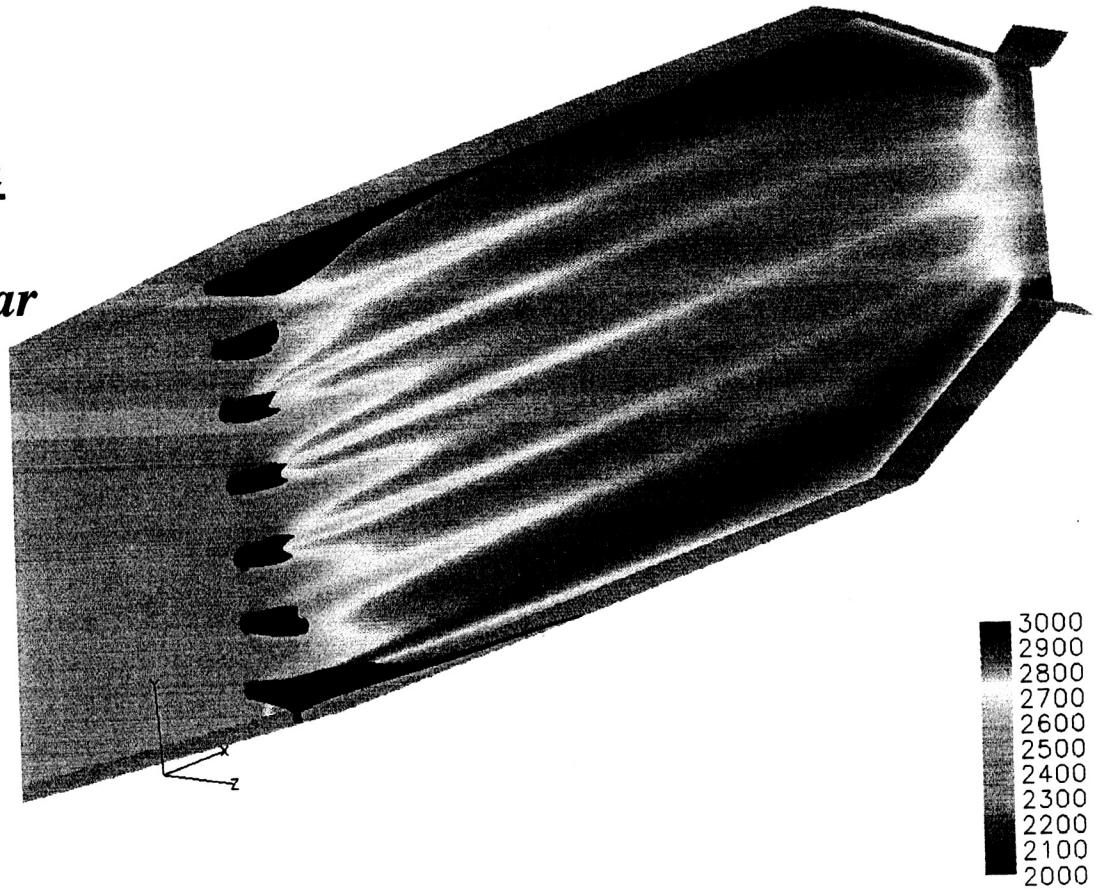


Application to PSU RBCC Rig- Ram Combustion

Ram Section and Outlet Nozzle

Ram Injection and Combustion

- ***Blue surfaces are near-flame surfaces- note recirculation near wall***
- ***Static Temperature scale in K***



Performance of Chem and FDNS on PSU RBCC Rig

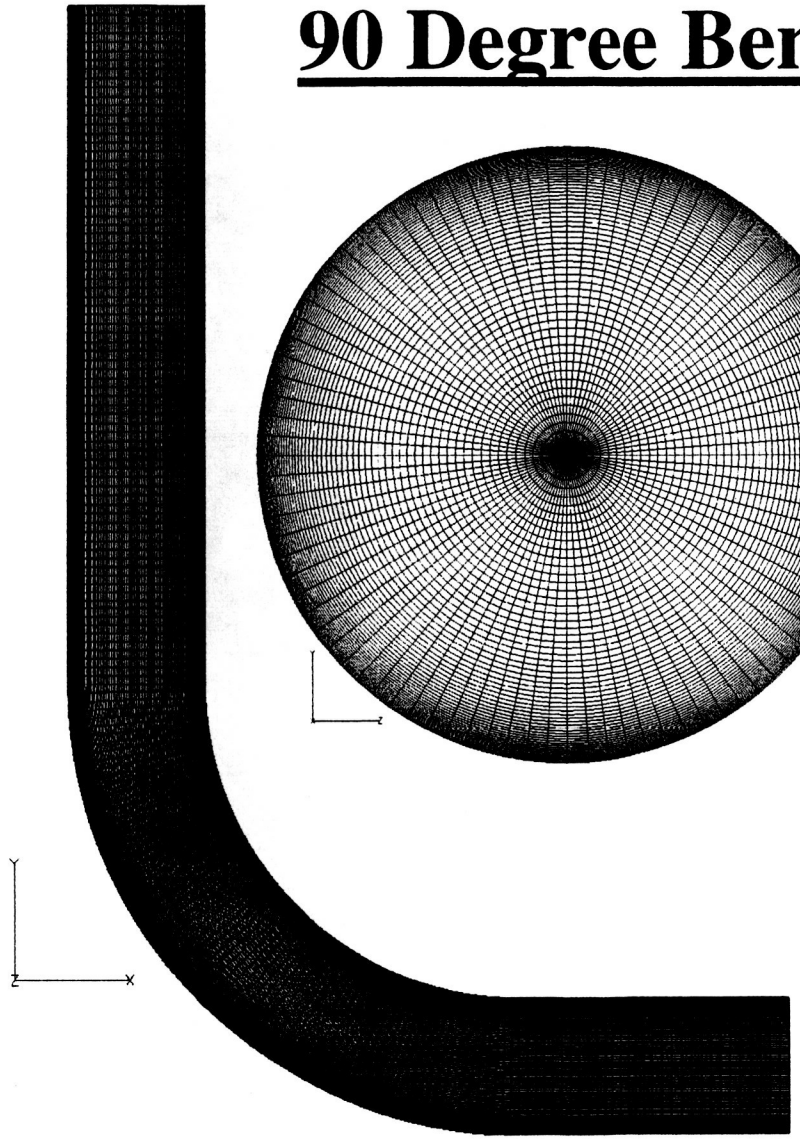
Chem (from quiescent)

- 0.6M grid points
- 10 hours wall clock using 32 CPUS
- 320 CPU days total effort
- Max possible CPUs for quality result=?
- *There is some evidence that too conservative timestep settings were used.*

FDNS (from restart)

- 0.5M grid points
- 6 days wall clock using 8 CPUs
- 48 CPU days total effort
- Max possible CPUs for quality result=8, due to grid constraints.

90 Degree Bend Benchmark Comparison



- Comparison with published data
- Laser velocimetry data
  - Velocity contours at several locations
- Static pressure along walls
- Re = 43,000 (turbulent flow)
- Operating fluid – water
- CHEM grid density of (185x93x61)

Reference:

Enayet, M. M., Gibson, M. M., Taylor, A. M. K. P. and Yianneskis, M. ``Laser-Doppler Measurements of Laminar and Turbulent Flow in a Pipe Bend,'' *Int. J. Heat & Fluid Flow*, 1982, Vol. 3, pp. 213-219.

90 Degree Bend Benchmark Comparison

Chem is strictly a perfect gas code, How do we approximate liquid water using a perfect gas model?

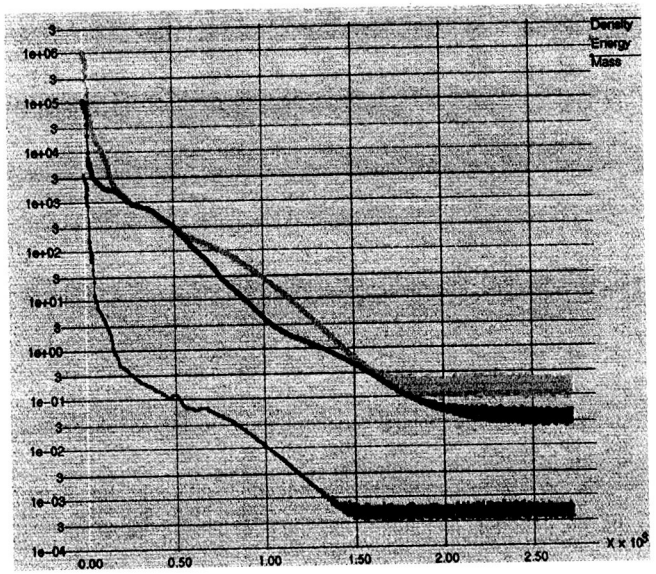
- **Choose a large gauge pressure such that $\Delta\rho/\rho$ is small and find the molecular weight to match density of liquid water at gauge pressure. Specify the transport properties of liquid water.**
- **We chose Pgauge=100psia which resulted in a molecular weight of 3523 kg/kmol**
- **For the simulation shown, $\Delta\rho$ was 996 to 998, indeed $\Delta\rho/\rho$ is quite small (0.002)**

90 Degree Bend Benchmark Comparison

Solution Details

- Used 12 CPUs (R10K@250MHZ)
- Completed 2600 iterations in 72 hours
- Practical convergence was achieved after 36 hours (1100 iterations)
- 6 to 7 orders of magnitude reduction in residuals
- Computational Domain mass conservation achieved within 0.001%

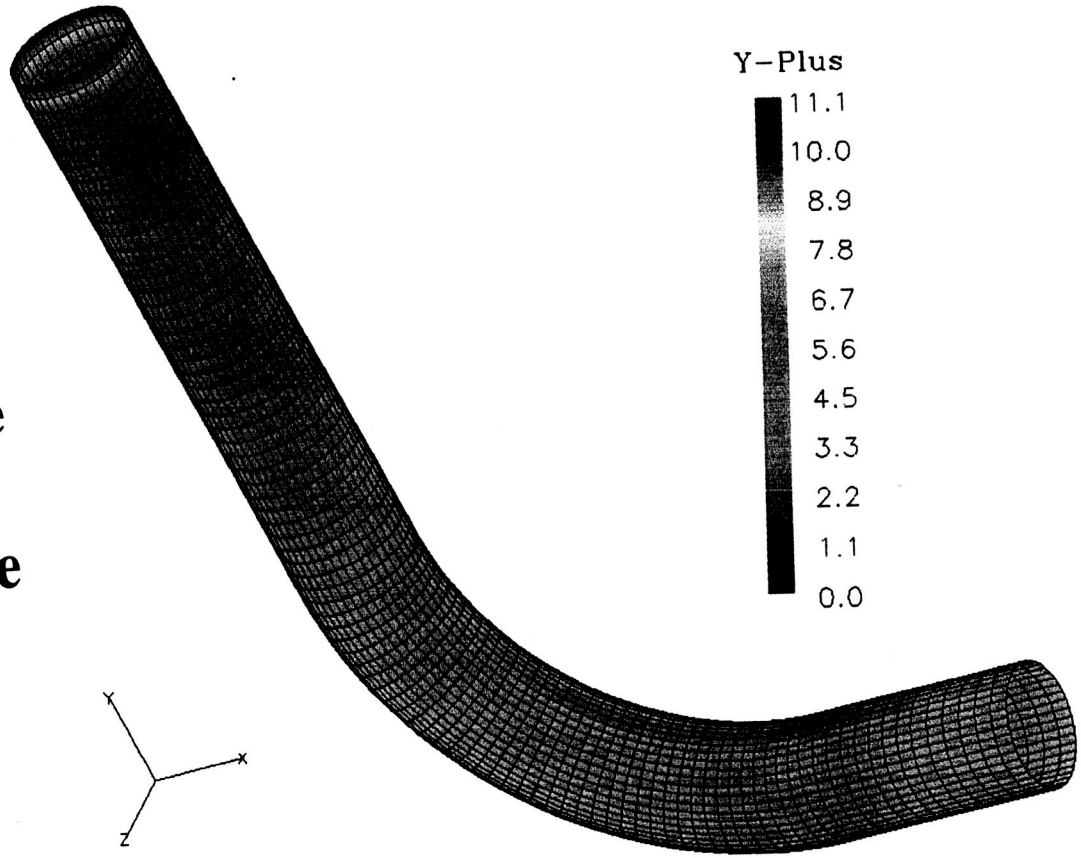
Residuals



90 Degree Bend Benchmark Comparison

Y+ Values

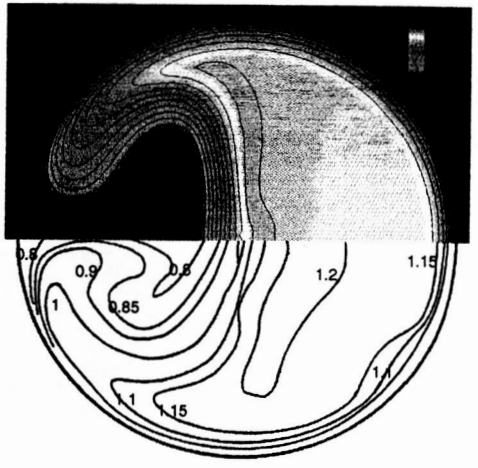
- Most gridpoints are within a Y+ of 6
- Every other gridline shown



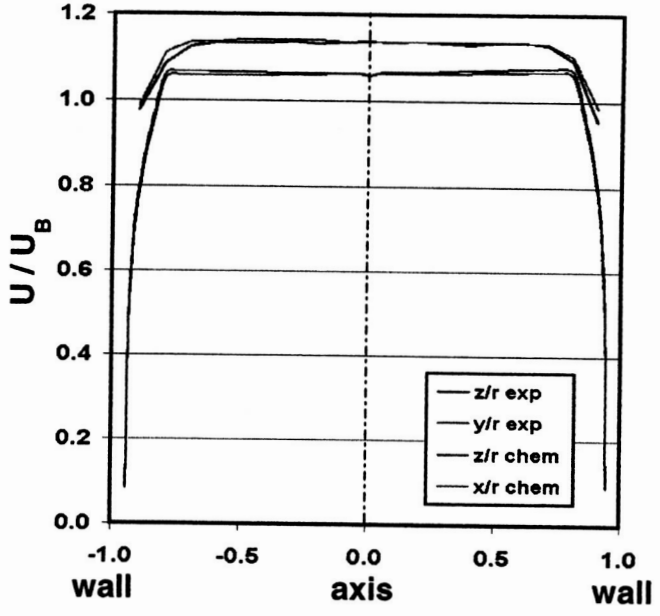
Velocity Distribution

CFD

Expt



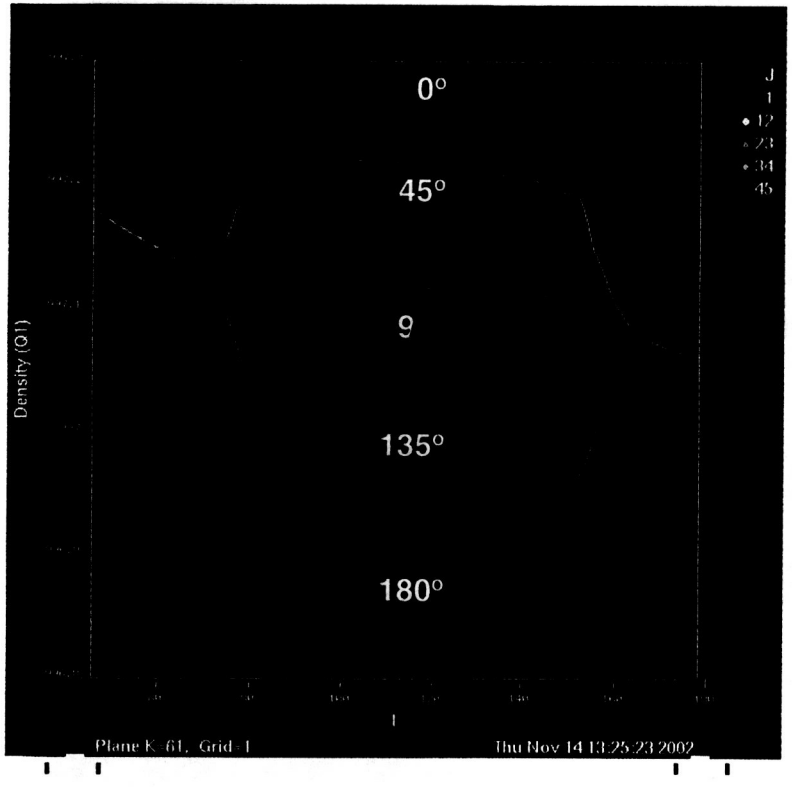
1-dia downstream of curve

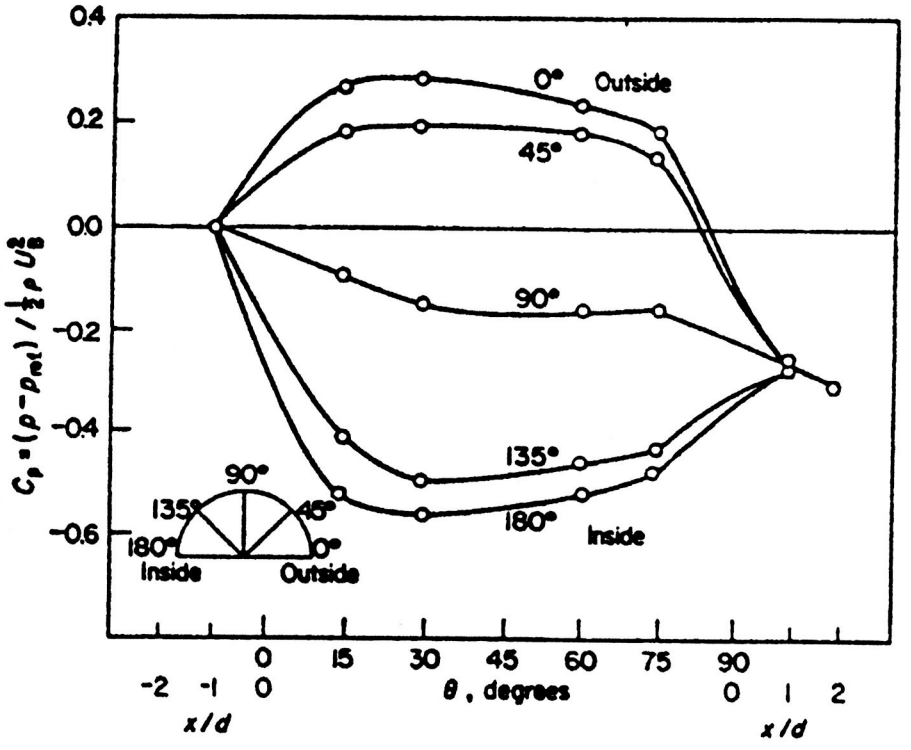


Note:

•A Slug Flow velocity distribution was applied at the duct inlet

Wall Static Pressure Variation





CFD

Experiment

Summary and Future Work

Positive Features

- **The additional effort required to execute in parallel verses serial is almost non-existent**
- **The Loci-Chem application can use efficiently more CPUs than the existing CFD tool (FDNS)**
- **The Loci-Chem application is very stable with respect to finite-rate chemistry, no reduction in timestep is required**
- **Loci-Chem supports structured, hybrid, and unstructured grids effortlessy though the Cobalt grid format**

Summary and Future Work

Negative Features

- **Mass fraction undershoots, temperature overshoots**
- **No fixed-mass inflow boundary condition**
- **No current support for non-collision-type chemical reaction rates (global or quasi-global models not yet supported)**
- **Very inefficient file I/O during parallel startup**
- **User is required to write conversions tools to allow post-processing with commercial tools (Fieldview, Ensight, etc)**

Summary and Future Work

General Difficulties

- **No one (here) has a LOT of experience creating hybrid grids**
- **Gridgen has issues with writing Cobalt grid format, bugs have been reported to Pointwise. (Half of all grids attempted will not write out properly)**
- **Having a coarse transition from structured to unstructured grids can be problematic. It is not easy to refine in a particular section of an unstructured grid.**

Summary and Future Work

Future Efforts

- **Chem will be applied to the PSU RBCC rig in a systematic fashion, attempting to benchmark the code with 6 different configurations *(JPC 2003 abstract submitted)***
- **Chem will be applied to more benchmark problems in an effort to establish a validation suite of problems**
- **We are currently funding and hope to continue to fund efforts to both increase maturity and add new features to the Loci-Chem CFD code (multi-disciplinary, real fluids, etc)**